STN Structure Search (Registry/Caplus)

L1 STRUCTURE UPLOADED

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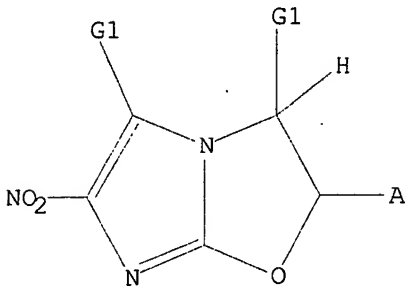
L1 STR



G1 H,Me

Structure attributes must be viewed using STN Express query preparation.

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FULL SCREEN SEARCH COMPLETED - 3098 TO ITERATE

100.0% PROCESSED 3098 ITERATIONS 2893 ANSWERS
SEARCH TIME: 00.00.01

L2 2893 SEA SSS FUL L1

=> fil caplus
COST IN U.S. DOLLARS

	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	166.94	167.15

FILE 'CAPLUS' ENTERED AT 17:32:52 ON 01 NOV 2006
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FILE COVERS 1907 - 1 Nov 2006 VOL 145 ISS 19
FILE LAST UPDATED: 31 Oct 2006 (20061031/ED)

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They are available for your review at:

http://www.cas.org/infopolicy.html

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L3 15 L2

=> d ibib abs 1-15

L3 ANSWER 1 OF 15 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2006:304659 CAPLUS <<LOGINID::20061101>>
DOCUMENT NUMBER: 145:39709
TITLE: Trends and advances in antituberculosis agents
AUTHOR(S): Lu, Yu; Duan, Lianshan
CORPORATE SOURCE: Beijing Tuberculosis and Thoracic Tumor Research Institute, Beijing, 101149, Peop. Rep. China
SOURCE: Zhongguo Kangshengsu Zazhi (2005), 30(4), 250-253
CODEN: ZKZAEY; ISSN: 1001-8689
PUBLISHER: Zhongguo Kangshengsu Zazhishe
DOCUMENT TYPE: Journal; General Review
LANGUAGE: Chinese
AB A review on the trends and advances in antituberculosis agents.

L3 ANSWER 2 OF 15 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2006:94067 CAPLUS <<LOGINID::20061101>>
DOCUMENT NUMBER: 144:346724
TITLE: Identification of a nitroimidazo-oxazine-specific protein involved in PA-824 resistance in Mycobacterium tuberculosis
AUTHOR(S): Manjunatha, Ujjini H.; Boshoff, Helena; Dowd, Cynthia S.; Zhang, Liang; Albert, Thomas J.; Norton, Jason E.; Daniels, Lacy; Dick, Thomas; Pang, Siew Siew; Barry, Clifton E., III
CORPORATE SOURCE: Tuberculosis Research Section, National Institute of Allergy and Infectious Diseases, Rockville, MD, 20852, USA
SOURCE: Proceedings of the National Academy of Sciences of the United States of America (2006), 103(2), 431-436
CODEN: PNASA6; ISSN: 0027-8424
PUBLISHER: National Academy of Sciences
DOCUMENT TYPE: Journal
LANGUAGE: English
AB PA-824 is a promising new compound for the treatment of tuberculosis that is currently undergoing human trials. Like its progenitors metronidazole and CGI-17341, PA-824 is a prodrug of the nitroimidazole class, requiring bioreductive activation of an aromatic nitro group to exert an antitubercular effect. The authors have confirmed that resistance to PA-824 (a nitroimidazo-oxazine) and CGI-17341 (a nitroimidazo-oxazole) is most commonly mediated by loss of a specific glucose-6-phosphate dehydrogenase (FGD1) or its deazaflavin cofactor F420, which together provide electrons for the reductive activation of this class of mols. Although FGD1 and F420 are necessary for sensitivity to these compds., they are not sufficient and require addnl. accessory proteins that directly interact with the nitroimidazole. To understand more proximal events in the reductive activation of PA-824, the authors examined mutants that were wild-type for both FGD1 and F420 and found that, although these mutants had acquired high-level resistance to PA-824 (and another nitroimidazo-oxazine), they retained sensitivity to CGI-17341 (and a related nitroimidazo-oxazole). Microarray-based comparative genome sequencing of these mutants identified lesions in Rv3547, a conserved

hypothetical protein with no known function. Complementation with intact Rv3547 fully restored sensitivity to nitroimidazo-oxazines and restored the ability of Mtb to metabolize PA-824. These results suggest that the sensitivity of Mtb to PA-824 and related compds. is mediated by a protein that is highly specific for subtle structural variations in these bicyclic nitroimidazoles.

REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 3 OF 15 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2005:1262333 CAPLUS <<LOGINID::20061101>>
DOCUMENT NUMBER: 144:22949
TITLE: Preparation of 2,3-dihydro-6-nitroimidazo[2,1-b]oxazoles as antibacterial agents
INVENTOR(S): Tsubochi, Hidetsugu; Sasaki, Hirofumi; Kuroda, Hideaki; Itotani, Motohiro; Hasegawa, Takeshi; Haraguchi, Yoshikazu; Kuroda, Takeshi; Matsuzaki, Takayuki; Tai, Kuninori; Komatsu, Makoto; Matsumoto, Makoto; Hashizume, Hiroyuki; Tomishige, Tatsuo; Seike, Yuji; Kawasaki, Masanori; Sumida, Takumi; Miyamura, Shin; Oguro, Kinue; Tanaka, Kazuho; Takemura, Isao
PATENT ASSIGNEE(S): Ohtsuka Pharmaceutical Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 1050 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
JP 2005330266	A2	20051202	JP 2005-113726		20050411
PRIORITY APPLN. INFO.:			JP 2004-114975	A	20040409
			JP 2004-125055	A	20040421

OTHER SOURCE(S): MARPAT 144:22949
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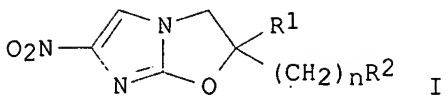

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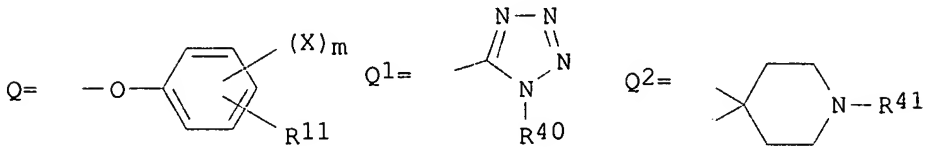

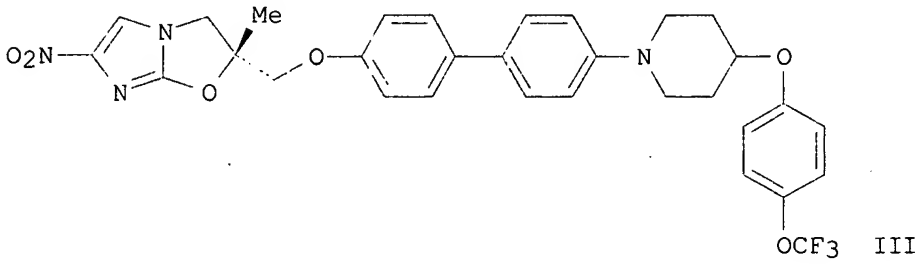

III

AB The title compds. [I; wherein R1 = H, C1-6 alkyl; n = an integer of 0-6; R2 = OR3, SR5, CO2R6, O2CNR7R8, Q, NR19R20, Q1; wherein R3 = H, C1-6 alkoxy, C1-6 alkoxy-C1-6 alkyl, (un)substituted phenyl-C1-6 alkoxy, biphenylyl-C1-6 alkoxy, phenyl-C2-6 alkenyl, C1-6 alkylsulfonyl, etc.; R5 = tetrazolyl or phenyltetrazolyl optionally substituted by halo or C1-6 alkyl on phenyl; R6 = C1-6 alkyl; R7, R8 = H, C1-8 alkyl, halo-C1-6 alkyl, C1-6 alkoxycarbonyl-C1-6 alkyl, C3-8 cycloalkyl, phenyl-C1-6 alkyl, Ph, naphthyl, pyridyl, etc.; X = halo, amino-C1-6 alkyl, C1-6 alkylamino-C1-6 alkyl; R11 = H, C1-6 alkyl, halo-C1-6 alkyl, C1-6 alkoxy, halo-C1-6 alkoxy, etc.; m = an integer of 0-3; R40 = C1-6 alkyl, Ph, halophenyl; or R1 and -(CH2)nR2 may be united via a nitrogen atom to form together with the adjacent carbon atom a spiro ring represented by the general formula Q2; wherein R41 = H, C1-6 alkyl, phenyl-C1-6 alkyl, biphenylyl-C1-6 alkyl, (un)substituted Ph, etc.] or optical isomers thereof or pharmacol. acceptable salts thereof are prepared These compds. exhibit excellent bactericidal activity against Tubercle bacillus, multiple drug resistant T. bacillus, and atypical acid-fast bacteria, and are useful as antitubercular agents. Thus, 0.43 g (S)-1-(2-chloro-4-nitroimidazol-1-yl)-2-methyl-3-[4-(4-trifluoromethoxyphenyl)piperazin-1-yl]propan-2-ol and 0.22 g 2-chloro-4-nitro-1H-imidazole were suspended in 4 mL MeCN, treated with 0.17 g NaHCO3, and refluxed for 9 h to give 31% (S)-1-(2-chloro-4-nitroimidazol-1-yl)-2-methyl-3-[4-(4-trifluoromethoxyphenyl)piperazin-1-yl]propan-1-ol which (5.85 g) was dissolved in 150 mL THF, treated with 0.66 g NaH under ice-cooling and refluxed for 6 h to give 48% (S)-2-[[4-(4-trifluoromethoxyphenyl)piperazin-1-yl]methyl]-2-methyl-6-nitro-2,3-dihydroimidazo[2,1-b]oxazole (II). II and compound (III) showed min. inhibitory concentration of 0.024 and 0.0015 μg/mL, resp., against Mycobacterium tuberculosis H37Rv.

L3 ANSWER 4 OF 15 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2005:1075755 CAPLUS <<LOGINID::20061101>>
DOCUMENT NUMBER: 143:367079
TITLE: Method of producing aminophenol compounds

INVENTOR(S): Kiyokawa, Hiroshi; Aki, Shinji
PATENT ASSIGNEE(S): Otsuka Pharmaceutical Co., Ltd., Japan
SOURCE: PCT Int. Appl., 66 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2005092832	A1	20051006	WO 2005-JP6408		20050325
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW					
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG					
AU 2005226409	A1	20051006	AU 2005-226409		20050325
JP 2005306866	A2	20051104	JP 2005-89215		20050325
PRIORITY APPLN. INFO.:			JP 2004-89652	A	20040325
			WO 2005-JP6408	W	20050325

OTHER SOURCE(S): CASREACT 143:367079; MARPAT 143:367079

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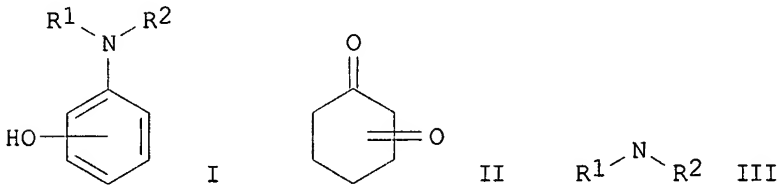

AB The present invention provides an industrially advantageous method of producing aminophenol compds. represented by the formula (I) by a simple and easy procedure at a high yield and a high purity. The present invention provides a method of producing an aminophenol compound represented by the formula (I): (wherein each of R1 and R2, which may be the same or different, is a hydrogen atom, a substituted or unsubstituted lower alkyl group or the like; R1 and R2, taken together with the adjacent nitrogen atom, may form a 5- or 6-membered heterocycle with or without other intervening heteroatoms; the heterocycle may be substituted by 1 to 3 substituents selected from the group consisting of a hydroxyl group, a substituted or unsubstituted lower alkyl group, a substituted or unsubstituted aryl group, a substituted or unsubstituted aryloxy group and the like; and the hydroxyl group in the formula (I) is substituted on the 2- or 4-position to the amino group on the Ph ring), which comprises allowing a cyclohexanedione compound represented by the formula (II) to react with an amine compound represented by the formula (III) (wherein R1 and R2 are as defined above), under a neutral or basic condition.

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 5 OF 15 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2005:409528 CAPLUS <<LOGINID::20061101>>
DOCUMENT NUMBER: 142:463728
TITLE: Preparation of 2,3-dihydro-6-nitroimidazo[2,1-b]oxazoles for the treatment of tuberculosis
INVENTOR(S): Tsubouchi, Hidetsugu; Sasaki, Hirofumi; Itotani, Motohiro; Haraguchi, Yoshikazu; Miyamura, Shin; Matsumoto, Makoto; Hashizume, Hiroyuki; Tomishige, Tatsuo; Kawasaki, Masanori; Ohguro, Kinue; Sumida, Takumi; Hasegawa, Takeshi; Tanaka, Kazuho; Takemura, Isao
PATENT ASSIGNEE(S): Otsuka Pharmaceutical Co., Ltd., Japan
SOURCE: PCT Int. Appl., 941 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005042542	A1	20050512	WO 2004-JP16492	20041029
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2004285811	A1	20050512	AU 2004-285811	20041029
CA 2539335	AA	20050512	CA 2004-2539335	20041029
EP 1678185	A1	20060712	EP 2004-793412	20041029
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK				
JP 2005320316	A2	20051117	JP 2004-318005	20041101

PRIORITY APPLN. INFO.:
JP 2003-373206 A 20031031
JP 2004-111720 A 20040406
WO 2004-JP16492 W 20041029

OTHER SOURCE(S): MARPAT 142:463728
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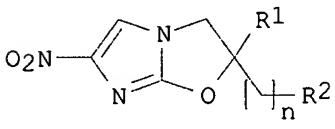

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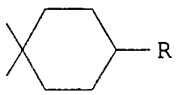


II

AB The title compds. I [R1 = H, alkyl; n = 0-6; R1 and (CH2)nR2, together

with the adjacent carbon atom, may form a spiro ring represented by II (wherein R = substituted piperidyl); R2 = benzothiazolyloxy, quinolyloxy, pyridyloxy, etc.] which have an excellent bactericidal action against Mycobacterium tuberculosis, multi-drug-resistant Mycobacterium tuberculosis, and atypical acid-fast bacteria, were prepared and formulated. Thus, reacting (R)-2-chloro-1-(2-methyl-2-oxiranylmethyl)-4-nitro-1H-imidazole with 6-hydroxy-2-[4-(4-trifluoromethoxybenzyl)piperazin-1-yl]benzothiazole in the presence of NaH in DMF afforded 33% (R)-2-methyl-6-nitro-2-{2-[4-(4-trifluoromethoxybenzyl)piperazin-1-yl]benzothiazol-6-yloxymethyl}-2,3-dihydroimidazo[2,1-b]oxazole which showed MIC of 0.2 μg/mL in antibacterial test against M. tuberculosis Kurono in 7H11 medium.

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

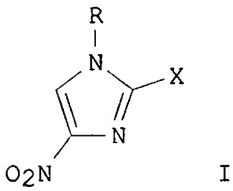
L3 ANSWER 6 OF 15 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:525386 CAPLUS <<LOGINID::20061101>>
DOCUMENT NUMBER: 141:199295
TITLE: Research advances in anti-tuberculosis drugs
AUTHOR(S): Wang, Wei; Jin, Guan-fu
CORPORATE SOURCE: Tuberculosis Research Center, 309th Hospital of PLA, Beijing, 100091, Peop. Rep. China
SOURCE: Yiyao Daobao (2004), 23(3), 131-134
CODEN: YDIAAL; ISSN: 1004-0781
PUBLISHER: Yiyao Daobao Zazhishe
DOCUMENT TYPE: Journal; General Review
LANGUAGE: Chinese
AB A review. Research advances in anti-tuberculosis drugs is reviewed including newly developed tuberculostatics such as ofloxacin, ciprofloxacin, levofloxacin, sparfloxacin, moxifloxacin, rifapentine, rifabutin, KRM-1648, isepamicin, paromomycin, enviomycin, CGI-17341, trifluoperazine, gangamicin, thiolactomycin, and DUP-721 etc. as well as pharmaceutical natural products with examples.

L3 ANSWER 7 OF 15 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:354918 CAPLUS <<LOGINID::20061101>>
DOCUMENT NUMBER: 140:375169
TITLE: Process for preparation of 4-nitroimidazole derivatives
INVENTOR(S): Goto, Fumitaka; Takemura, Noriaki; Otani, Tadaaki; Hasegawa, Takeshi; Tsubouchi, Hidetsugu; Utsumi, Naoto; Fujita, Shigekazu; Kuroda, Hideaki; Shitsuta, Takuya; Sasaki, Hirofumi
PATENT ASSIGNEE(S): Otsuka Pharmaceutical Co., Ltd., Japan
SOURCE: PCT Int. Appl., 127 pp.
CODEN: PIXXD2
DOCUMENT TYPE: ~~Patent~~
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: ~~1~~
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004035547	A1	20040429	WO 2003-JP13134	20031014
W: AU, BR, BY, CA, CN, EG, ID, IN, KR, MX, PH, PL, RU, SG, UA, US, VN, ZA				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR				
CA 2494710	AA	20040429	CA 2003-2494710	20031014

AU 2003301282	A1	20040504	AU 2003-301282		20031014
BR 2003013566	A	20050621	BR 2003-13566		20031014
EP 1553088	A1	20050713	EP 2003-756610		20031014
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, SK					
CN 1692103	A	20051102	CN 2003-80100667		20031014
JP 2004269500	A2	20040930	JP 2003-354575		20031015
US 2006079697	A1	20060413	US 2005-523008		20050201
PRIORITY APPLN. INFO.:			JP 2002-299896	A	20021015
			JP 2003-37914	A	20030217
			WO 2003-JP13134	W	20031014

OTHER SOURCE(S): MARPAT 140:375169
GI



I

AB This invention pertains to a method for producing 4-nitroimidazole derivs. with general formula of I [wherein R = H, alkoxyalkyl, phenylalkoxyalkyl, cyanoalkyl, (un)substituted phenylalkyl, or alkyl, etc.; X = halo or SOnR1; n = 0-2; R1 = (un)substituted Ph; with a proviso]. For example, 2-bromo-1-(methoxymethyl)-4-nitroimidazole (preparation given) was treated with 5N aqueous HCl in MeOH to give 2-bromo-4-nitroimidazole (66%). I are useful as intermediates for various medicines and agricultural chems., especially as intermediates for antitubercular agents.

REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

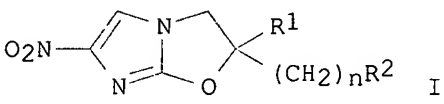
L3 ANSWER 8 OF 15 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:333722 CAPLUS <<LOGINID::20061101>>
DOCUMENT NUMBER: 140:357387
TITLE: Preparation of 2,3-dihydro-6-nitroimidazo[2,1-b]oxazoles as antibacterial agents
INVENTOR(S): Tsubouchi, Hidetsugu; Sasaki, Hirofumi; Kuroda, Hideaki; Itotani, Motohiro; Hasegawa, Takeshi; Haraguchi, Yoshikazu; Kuroda, Takeshi; Matsuzaki, Takayuki; Tai, Kuninori; Komatsu, Makoto; Matsumoto, Makoto; Hashizume, Hiroyuki; Tomishige, Tatsuo; Seike, Yuji; Kawasaki, Masanori; Sumida, Takumi; Miyamura, Shin
PATENT ASSIGNEE(S): Otsuka Pharmaceutical Co., Ltd., Japan
SOURCE: PCT Int. Appl., 1084 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2004033463	A1	20040422	WO 2003-JP13070		20031010
W: AU, BR, BY, CA, CN, EG, ID, IN, KR, MX, PH, PL, RU, SG, UA, US, VN, ZA					
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR					
CA 2497569	AA	20040422	CA 2003-2497569		20031010
AU 2003272979	A1	20040504	AU 2003-272979		20031010
BR 2003014344	A	20050712	BR 2003-14344		20031010
EP 1555267	A1	20050720	EP 2003-754085		20031010
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, SK					
CN 1705670	A	20051207	CN 2003-80101750		20031010
JP 2004149527	A2	20040527	JP 2003-353868		20031014
US 2006094767	A1	20060504	US 2005-530429		20050406
PRIORITY APPLN. INFO.:			JP 2002-298259	A	20021011
			WO 2003-JP13070	W	20031010

Instant App.

OTHER SOURCE(S): MARPAT 140:357387

GI



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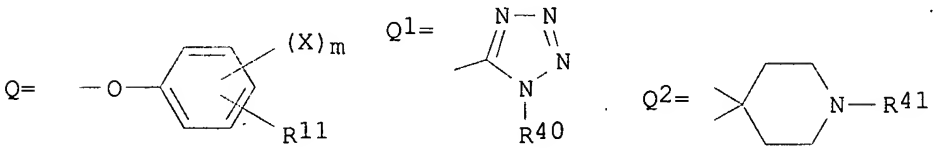

AB The title compds. [I; wherein R1 = H, C1-6 alkyl; n = an integer of 0-6; R2 = OR3, SR5, CO2R6, O2CNR7R8, Q, NR19R20, Q1; wherein R3 = H, C1-6 alkoxy, C1-6 alkoxy-C1-6 alkyl, (un)substituted phenyl-C1-6 alkoxy, biphenylyl-C1-6 alkoxy, phenyl-C2-6 alkenyl, C1-6 alkylsulfonyl, etc.; R5 = tetrazolyl or phenyltetrazolyl optionally substituted by halo or C1-6 alkyl on phenyl; R6 = C1-6 alkyl; R7, R8 = H, C1-8 alkyl, halo-C1-6 alkyl, C1-6 alkoxycarbonyl-C1-6 alkyl, C3-8 cycloalkyl, phenyl-C1-6 alkyl, Ph, naphthyl, pyridyl, etc.; X = halo, amino-C1-6 alkyl, C1-6 alkylamino-C1-6 alkyl; R11 = H, C1-6 alkyl, halo-C1-6 alkyl, C1-6 alkoxy, halo-C1-6 alkoxy, etc.; m = an integer of 0-3; R40 = C1-6 alkyl, Ph, halophenyl; or R1 and -(CH2)nR2 may be united via a nitrogen atom to form together with the adjacent carbon atom a spiro ring represented by the general formula Q2; wherein R41 = H, C1-6 alkyl, phenyl-C1-6 alkyl, biphenylyl-C1-6 alkyl, (un)substituted Ph, etc.] are prepared These compds. exhibit excellent bactericidal activity against Tubercle bacillus, multiple drug resistant T. bacillus, and atypical acid-fast bacteria, and are useful as antitubercular agents. Thus, 0.43 g (S)-1-(2-chloro-4-nitroimidazol-1-yl)-2-methyl-3-[4-(4-trifluoromethoxyphenyl)piperazin-1-yl]propan-2-ol and 0.22 g 2-chloro-4-nitro-1H-imidazole were suspended in 4 mL MeCN, treated with 0.17 g NaHCO3, and refluxed for 9 h to give 31% (S)-1-(2-chloro-4-nitroimidazol-1-yl)-2-methyl-3-[4-(4-trifluoromethoxyphenyl)piperazin-1-

yl]propan-1-ol which (5.85 g) was dissolved in 150 mL THF, treated with 0.66 g NaH under ice-cooling and refluxed for 6 h to give 48% (S)-2-[[4-(4-trifluoromethoxyphenyl)piperazin-1-yl]methyl]-2-methyl-6-nitro-2,3-dihydroimidazo[2,1-b]oxazole (II). II showed min. inhibitory concentration of 0.024 μg/mL against Mycobacterium tuberculosis H37Rv.
REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 9 OF 15 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:184650 CAPLUS <<LOGINID::20061101>>
DOCUMENT NUMBER: 140:375114
TITLE: 2,4-Dinitroimidazole: Microwave assisted synthesis and use in synthesis of 2,3-dihydro-6-nitroimidazo[2,1-b]oxazole analogues with antimycobacterial activity
AUTHOR(S): Bhaumik, Kankan; Akamanchi, K. G.
CORPORATE SOURCE: Chembiotek Research International Pvt. Ltd., Kolkata, 700 091, India
SOURCE: Journal of Heterocyclic Chemistry (2004), 41(1), 51-55
CODEN: JHTCAD; ISSN: 0022-152X
PUBLISHER: HeteroCorporation
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 140:375114
AB 2,4-Dinitroimidazole (I), an important starting material for nitroimidazooxazole and nitroimidazooxazine types of antitubercular agents was synthesized by rearrangement of 1,4-dinitroimidazole under microwave irradiation Various new nitroimidazooxazoles analogs were prepared from I and were tested preliminarily against Mycobacterium tuberculosis, H37Rv strain. Some were found to be active.
REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 10 OF 15 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2000:461733 CAPLUS <<LOGINID::20061101>>
DOCUMENT NUMBER: 133:171806
TITLE: A small-molecule nitroimidazopyran drug candidate for the treatment of tuberculosis
AUTHOR(S): Stover, C. Kendall; Warrener, Paul; VanDevanter, Donald R.; Sherman, David R.; Arain, Taraq M.; Langhorne, Michael H.; Anderson, Scott W.; Towell, J. Andrew; Yuan, Ying; McMurray, David N.; Krelswirth, Barry N.; Barry, Clifton E.; Baker, William R.
CORPORATE SOURCE: PathoGenesis Corporation, Seattle, WA, 98119, USA
SOURCE: Nature (London) (2000), 405(6789), 962-966
CODEN: NATUAS; ISSN: 0028-0836
PUBLISHER: Nature Publishing Group
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Mycobacterium tuberculosis, which causes tuberculosis, is the greatest single infectious cause of mortality worldwide, killing roughly; two million people annually. Ests. indicate that one-third of the world population is infected with latent M. tuberculosis. The synergy between tuberculosis and the AIDS epidemic, and the surge of multidrug-resistant clin. isolates of M. tuberculosis have reaffirmed tuberculosis as a primary public health threat. However, new antitubercular drugs with new mechanisms of action have not been developed in over thirty years. Here we report a series of compds. containing a nitroimidazopyran nucleus that possess antitubercular activity. After activation by a mechanism dependent on M. tuberculosis F420 cofactor, nitroimidazopyrans inhibited

the synthesis of protein and cell wall lipid. In contrast to current antitubercular drugs, nitroimidazopyrans exhibited bactericidal activity against both replicating and static M. tuberculosis. Lead compound PA-824 showed potent bactericidal activity against multidrug-resistant M. tuberculosis and promising oral activity in animal infection models. We conclude that nitroimidazopyrans offer the practical qualities of a small mol. with the potential for the treatment of tuberculosis.

REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 11 OF 15 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1993:209297 CAPLUS <<LOGINID::20061101>>
DOCUMENT NUMBER: 118:209297
TITLE: In vitro and in vivo activities of the nitroimidazole CGI 17341 against Mycobacterium tuberculosis
AUTHOR(S): Ashtekar, Dilip R.; Costa-Perira, Rabi; Nagrajan, K.; Vishvanathan, N.; Bhatt, Arun D.; Rittel, Werner
CORPORATE SOURCE: Pharm. Res. Cent., Hindustan Ciba-Geigy, Bombay, 30206, India
SOURCE: Antimicrobial Agents and Chemotherapy (1993), 37(2), 183-6
CODEN: AMACCQ; ISSN: 0066-4804
DOCUMENT TYPE: Journal
LANGUAGE: English
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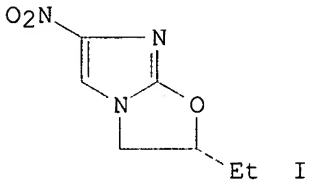

I

AB CGI 17341 (2-ethyl-5-nitro-2,3-dihydro[2-1b]imidazooxazole, I)) is a novel orally active representative of the 5-nitroimidazole series of antimicrobial agents. At concns. of 0.1-0.3 μg/mL, I inhibited the drug-susceptible and multidrug-resistant strains of M. tuberculosis. I had no cross-resistance with isoniazid, rifampin, streptomycin, or ethambutol. While the in vitro activity of I against M. tuberculosis was comparable to those of isoniazid and rifampin, it was superior to those of streptomycin, ciprofloxacin, norfloxacin, and oxazolidinone DuP 721. The MIC of I was not affected when the pH of the medium was decreased from 6.8 to 5.6, while 4-6-fold increases in the MICs of ciprofloxacin and isoniazid were observed In mice infected with M. tuberculosis, the 50% ED for I was 7.7 mg/kg body weight (95% confidence limits, 3.5 and 10.27) when administered on days 11 and 12 postinfection. I gave a dose-dependent and significant increase in the survival time. I is a promising and novel antituberculosis compound with potent in vitro and in vivo activities.

L3 ANSWER 12 OF 15 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1990:423764 CAPLUS <<LOGINID::20061101>>
DOCUMENT NUMBER: 113:23764
TITLE: Nitroimidazoles. XXI. 2,3-Dihydro-6-nitroimidazo[2,1-b]oxazoles with antitubercular activity

AUTHOR(S): Nagarajan, Kuppuswamy; Shankar, Radhakrishnan Gowri; Rajappa, Srinivasachari; Shenoy, Sharada J.; Costa-Pereira, Raby
CORPORATE SOURCE: Res. Cent., Hindustan Ciba-Geigy Ltd., Bombay, 400 063, India
SOURCE: European Journal of Medicinal Chemistry (1989), 24(6), 631-3
CODEN: EJMCA5; ISSN: 0223-5234
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 113:23764
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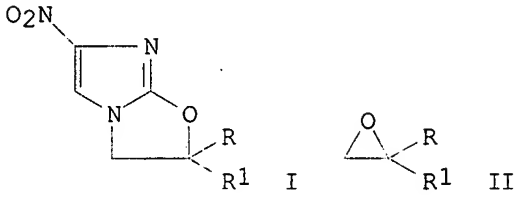
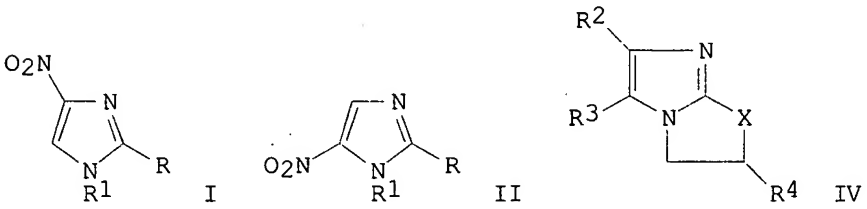


AB Title compds. I (R = alkyl, CH2Cl, CH2Br, CCl3, Ph, PhOCH2, etc., R1 = H, alkyl, CH2Cl, CH2Br, etc.) were prepared by reaction of 2,4-dinitroimidazole with oxiranes II. I showed antitubercular activity in mice.

L3 ANSWER 13 OF 15 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1984:611044 CAPLUS <<LOGINID::20061101>>
DOCUMENT NUMBER: 101:211044
TITLE: Nitroimidazoles: part XX - reactions of 2,4-dinitroimidazole with 2-haloethanols, 3-chloropropionitrile and propylene oxide
AUTHOR(S): Nagarajan, K.; Shenoy, S. J.
CORPORATE SOURCE: Res. Cent., CIBA-GEIGY, Bombay, 400 063, India
SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1984), 23B(4), 363-8
CODEN: IJSBDB; ISSN: 0376-4699
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 101:211044
GI



AB 2,4-Dinitroimidazoles I (R = NO2, R1 = Me) reacted with BrCH2CH2OH,

ClCH2CH2OH, Cl(CH2)3OH or ClCH2CH2CN to give I (R = Br, Cl; R1 = H, Me). Methylation of I (R = Br, Cl; R1 = H) gave isomeric imidazoles I and II (R = Br, Cl; R1 = Me). Other products from the reaction of I (R = NO2, R1 = H) (III) and ClCH2CH2CN were I (R = Cl, R1 = CH2CH2CN, CH2CH2CONH2) and cyclocondensation product pyrroloimidazole IV (R2 = NO2, R3 = R4 = H; X = CO). III reacted with propylene oxide to give imidazooxazoline IV (R2 = H, R3 = NO2, R4 = Me; X = O) and I (R = NO2, R1 = CH2CHMeOH, CHMeCH2OH), which (R1 = CH2CHMeOH) cyclized to give IV (R2 = NO2, R3 = H, R4 = Me; X = O). Propylene oxide and I (R = Cl, R1 = H) gave I and II (R = Cl, R1 = CH2CHMeOH), the latter of which cyclized to give IV (R2 = H, R3 = NO2, R4 = Me; X = O).

L3 ANSWER 14 OF 15 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1981:174982 CAPLUS <<LOGINID::20061101>>
DOCUMENT NUMBER: 94:174982
TITLE: Potential radiosensitizing agents. 2. Synthesis and biological activity of derivatives of dinitroimidazole with oxiranes
AUTHOR(S): Sehgal, Raj K.; Webb, Matthew W.; Agrawal, Krishna C.
CORPORATE SOURCE: Sch. Med., Tulane Univ., New Orleans, LA, 70112, USA
SOURCE: Journal of Medicinal Chemistry (1981), 24(5), 601-4
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 94:174982
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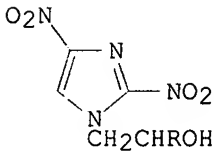
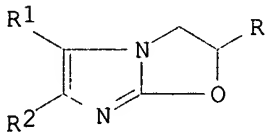


I



II

AB 1-Substituted 2,4-dinitroimidazole analogs were prepared and tested for their radiosensitizing ability for selectively sensitizing the hypoxic mammalian cells to the lethal effect of radiation. The reaction of 2,4(5)-dinitroimidazole with a variety of oxiranes upon heating in absolute EtOH yielded the expected 1-substituted 2,4-dinitroimidazoles I (R = H, Me, ClCH2, MeOCH2) as well as the novel isomeric nitroimidazooxazoles II (R1 = NO2, R2 = H; R2 = H, R1 = NO2) by intramol. cyclization. The results of radiosensitizing activity of these agents against hypoxic Chinese hamster cells (V-79) indicated that I were better sensitizers than II suggesting the necessity of the 2-nitro function in the mol. I (R = MeOCH2) was found to be the most effective radiosensitizer of this series.

L3 ANSWER 15 OF 15 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1980:163899 CAPLUS <<LOGINID::20061101>>
DOCUMENT NUMBER: 92:163899
TITLE: Novel nitroimidazo[2,1-b]oxazole formation from reaction of 2,4(5)-dinitroimidazole with oxiranes
AUTHOR(S): Sehgal, Raj K.; Agrawal, Krishna C.
CORPORATE SOURCE: Sch. Med., Tulane Univ., New Orleans, LA, 70112, USA
SOURCE: Journal of Heterocyclic Chemistry (1979), 16(7), 1499-500

CODEN: JHTCAD; ISSN: 0022-152X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 92:163899

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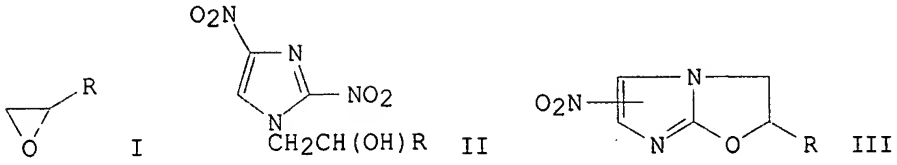


AB The reaction of 2,4-dinitroimidazole with oxiranes I gave imidazoles II and nitroimidazo[2,1-b]oxazoles III [NO2 at 5-position, 6-position; R = H, Me, CH2Cl, CH2OMe].

L3 ANSWER 7 OF 15 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:354918 CAPLUS <<LOGINID::20061101>>
DOCUMENT NUMBER: 140:375169
TITLE: Process for preparation of 4-nitroimidazole derivatives
INVENTOR(S): Goto, Fumitaka; Takemura, Noriaki; Otani, Tadaaki; Hasegawa, Takeshi; Tsubouchi, Hidetsugu; Utsumi, Naoto; Fujita, Shigekazu; Kuroda, Hideaki; Shitsuta, Takuya; Sasaki, Hirofumi
PATENT ASSIGNEE(S): Otsuka Pharmaceutical Co., Ltd., Japan
SOURCE: PCT Int. Appl., 127 pp.
CODEN: PIXXD2

same ✓

DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004035547	A1	20040429	WO 2003-JP13134	20031014
W: AU, BR, BY, CA, CN, EG, ID, IN, KR, MX, PH, PL, RU, SG, UA, US, VN, ZA				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR				
CA 2494710	AA	20040429	CA 2003-2494710	20031014
AU 2003301282	A1	20040504	AU 2003-301282	20031014
BR 2003013566	A	20050621	BR 2003-13566	20031014
EP 1553088	A1	20050713	EP 2003-756610	20031014
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, SK				
CN 1692103	A	20051102	CN 2003-80100667	20031014
JP 2004269500	A2	20040930	JP 2003-354575	20031015
US 2006079697	A1	20060413	US 2005-523008	20050201

10/14/03 filed after

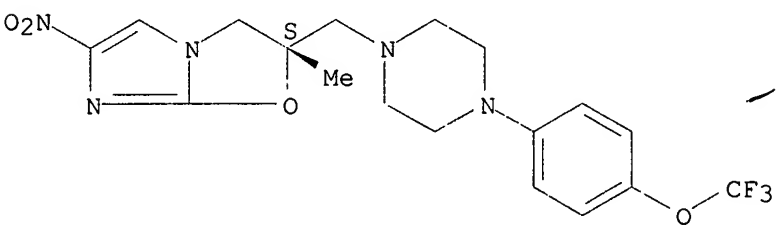
2/1/05

PRIORITY APPLN. INFO.:
JP 2002-299896 A 20021015
JP 2003-37914 A 20030217
WO 2003-JP13134 W 20031014

} after 10/11/02 (priority date)

OTHER SOURCE(S): MARPAT 140:375169
IT 681033-48-7P
RL: AGR (Agricultural use); BSU (Biological study, unclassified); IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(intermediate; preparation of nitroimidazole derivs.)
RN 681033-48-7 CAPLUS
CN Imidazo[2,1-b]oxazole, 2,3-dihydro-2-methyl-6-nitro-2-[[4-[4-(trifluoromethoxy)phenyl]-1-piperazinyl]methyl]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



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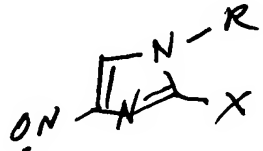
claim 1



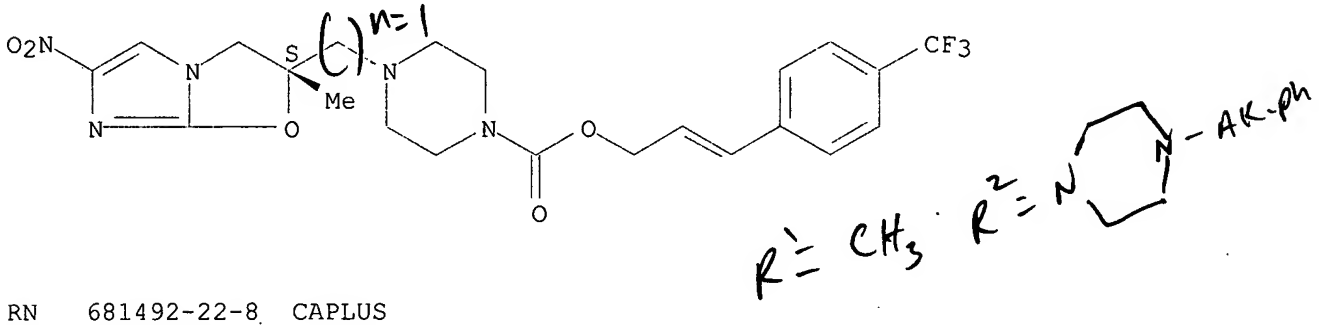
intermediates for

IT 681033-79-4P 681492-22-8P
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of nitroimidazole derivs.)

RN 681033-79-4 CAPLUS

CN 1-Piperazinecarboxylic acid, 4-[[(2S)-2,3-dihydro-2-methyl-6-nitroimidazo[2,1-b]oxazol-2-yl]methyl]-, 3-[4-(trifluoromethyl)phenyl]-2-propenyl ester (9CI) (CA INDEX NAME)

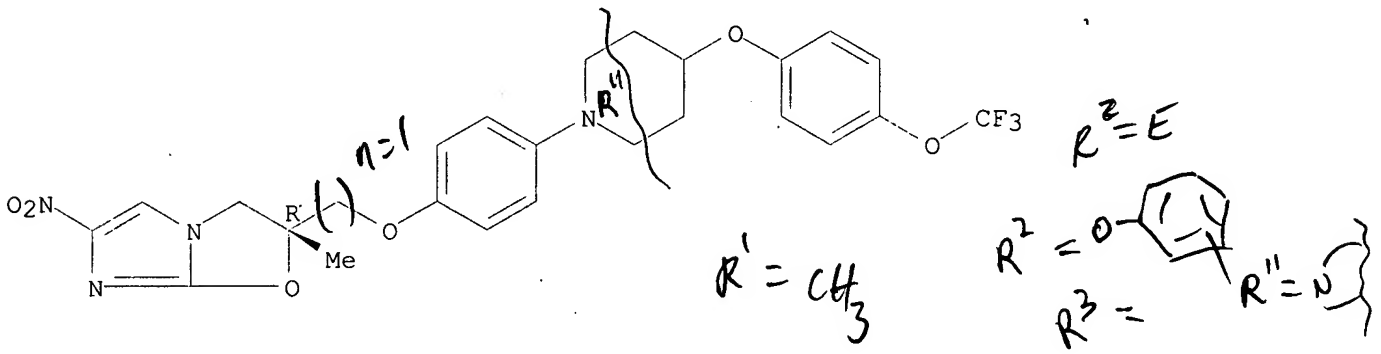
Absolute stereochemistry.
Double bond geometry unknown.



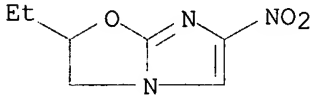
RN 681492-22-8 CAPLUS

CN Imidazo[2,1-b]oxazole, 2,3-dihydro-2-methyl-6-nitro-2-[[4-[4-[4-(trifluoromethoxy)phenoxy]-1-piperidinyl]phenoxy]methyl]-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 10 OF 15 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2000:461733 CAPLUS <<LOGINID::20061101>>
DOCUMENT NUMBER: 133:171806
TITLE: A small-molecule nitroimidazopyran drug candidate for the treatment of tuberculosis
AUTHOR(S): Stover, C. Kendall; Warrener, Paul; VanDevanter, Donald R.; Sherman, David R.; Arain, Taraq M.; Langhorne, Michael H.; Anderson, Scott W.; Towell, J. Andrew; Yuan, Ying; McMurray, David N.; Krelswirth, Barry N.; Barry, Clifton E.; Baker, William R.
CORPORATE SOURCE: PathoGenesis Corporation, Seattle, WA, 98119, USA
SOURCE: Nature (London) (2000), 405(6789), 962-966
CODEN: NATUAS; ISSN: 0028-0836
PUBLISHER: Nature Publishing Group
DOCUMENT TYPE: Journal
LANGUAGE: English
IT 127692-13-1, CGI-17341
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(a small-mol. nitroimidazopyran drug candidate for the treatment of tuberculosis)
RN 127692-13-1 CAPLUS
CN Imidazo[2,1-b]oxazole, 2-ethyl-2,3-dihydro-6-nitro- (9CI) (CA INDEX NAME)

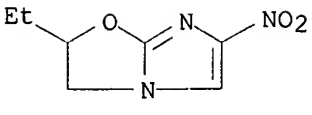


$R^2 \neq Me$

$R^1 = H$ X

REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 11 OF 15 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1993:209297 CAPLUS <<LOGINID::20061101>>
DOCUMENT NUMBER: 118:209297
TITLE: In vitro and in vivo activities of the nitroimidazole CGI 17341 against Mycobacterium tuberculosis
AUTHOR(S): Ashtekar, Dilip R.; Costa-Perira, Rabi; Nagrajan, K.; Vishvanathan, N.; Bhatt, Arun D.; Rittel, Werner
CORPORATE SOURCE: Pharm. Res. Cent., Hindustan Ciba-Geigy, Bombay, 30206, India
SOURCE: Antimicrobial Agents and Chemotherapy (1993), 37(2), 183-6
CODEN: AMACCQ; ISSN: 0066-4804
DOCUMENT TYPE: Journal
LANGUAGE: English
IT 127692-13-1, CGI 17341
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(Mycobacterium tuberculosis sensitivity to)
RN 127692-13-1 CAPLUS
CN Imidazo[2,1-b]oxazole, 2-ethyl-2,3-dihydro-6-nitro- (9CI) (CA INDEX NAME)



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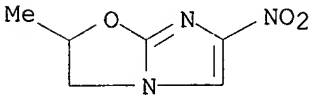
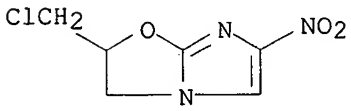
L3 ANSWER 12 OF 15 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1990:423764 CAPLUS <<LOGINID::20061101>>
DOCUMENT NUMBER: 113:23764
TITLE: Nitroimidazoles. XXI. 2,3-Dihydro-6-nitroimidazo[2,1-b]oxazoles with antitubercular activity
AUTHOR(S): Nagarajan, Kuppuswamy; Shankar, Radhakrishnan Gowri; Rajappa, Srinivasachari; Shenoy, Sharada J.; Costa-Pereira, Raby
CORPORATE SOURCE: Res. Cent., Hindustan Ciba-Geigy Ltd., Bombay, 400 063, India
SOURCE: European Journal of Medicinal Chemistry (1989), 24(6), 631-3
CODEN: EJMCA5; ISSN: 0223-5234
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 113:23764
IT 73332-75-9 73332-76-0 127692-13-1
127692-16-4 127692-17-5 127692-18-6
127692-19-7 127692-20-0 127692-21-1
127692-22-2 127692-23-3
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(tuberculostatic activity of)
RN 73332-75-9 CAPLUS
CN Imidazo[2,1-b]oxazole, 2,3-dihydro-2-methyl-6-nitro- (9CI) (CA INDEX NAME)



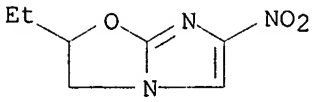
X

RN 73332-76-0 CAPLUS
CN Imidazo[2,1-b]oxazole, 2-(chloromethyl)-2,3-dihydro-6-nitro- (9CI) (CA INDEX NAME)



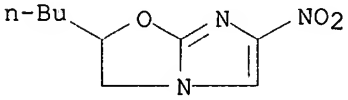
X $R^2 \neq X$

RN 127692-13-1 CAPLUS
CN Imidazo[2,1-b]oxazole, 2-ethyl-2,3-dihydro-6-nitro- (9CI) (CA INDEX NAME)

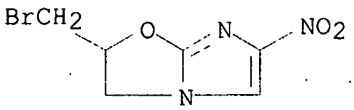


— same as #10

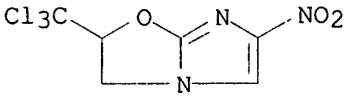
RN 127692-16-4 CAPLUS
CN Imidazo[2,1-b]oxazole, 2-butyl-2,3-dihydro-6-nitro- (9CI) (CA INDEX NAME)



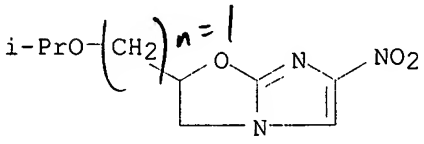
RN 127692-17-5 CAPLUS
CN Imidazo[2,1-b]oxazole, 2-(bromomethyl)-2,3-dihydro-6-nitro- (9CI) (CA INDEX NAME)



RN 127692-18-6 CAPLUS
CN Imidazo[2,1-b]oxazole, 2,3-dihydro-6-nitro-2-(trichloromethyl)- (9CI) (CA INDEX NAME)



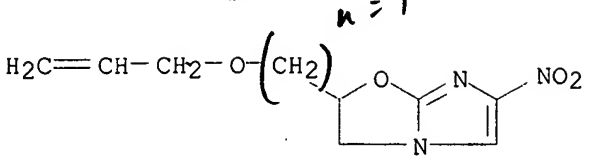
RN 127692-19-7 CAPLUS
CN Imidazo[2,1-b]oxazole, 2,3-dihydro-2-[(1-methylethoxy)methyl]-6-nitro- (9CI) (CA INDEX NAME)



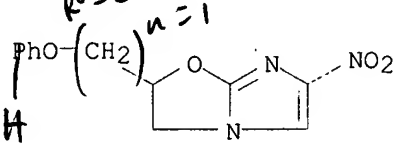
$R^2 = O\text{-}R^3$
$R^3 = i\text{-}Pr$

This is proviso (1) excluded cmpd

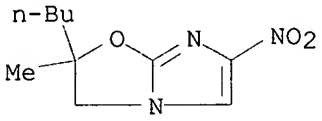
RN 127692-20-0 CAPLUS
CN Imidazo[2,1-b]oxazole, 2,3-dihydro-6-nitro-2-[(2-propenyloxy)methyl]- (9CI) (CA INDEX NAME)



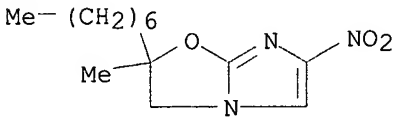
RN 127692-21-1 CAPLUS
CN Imidazo[2,1-b]oxazole, 2,3-dihydro-6-nitro-2-(phenoxymethyl)- (9CI) (CA INDEX NAME)



RN 127692-22-2 CAPLUS
CN Imidazo[2,1-b]oxazole, 2-butyl-2,3-dihydro-2-methyl-6-nitro- (9CI) (CA INDEX NAME)

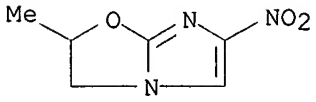


RN 127692-23-3 CAPLUS
CN Imidazo[2,1-b]oxazole, 2-heptyl-2,3-dihydro-2-methyl-6-nitro- (9CI) (CA INDEX NAME)



L3 ANSWER 13 OF 15 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1984:611044 CAPLUS <<LOGINID::20061101>>
DOCUMENT NUMBER: 101:211044
TITLE: Nitroimidazoles: part XX - reactions of 2,4-dinitroimidazole with 2-haloethanols, 3-chloropropionitrile and propylene oxide
AUTHOR(S): Nagarajan, K.; Shenoy, S. J.
CORPORATE SOURCE: Res. Cent., CIBA-GEIGY, Bombay, 400 063, India
SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1984), 23B(4), 363-8
CODEN: IJSBDB; ISSN: 0376-4699
DOCUMENT TYPE: Journal
LANGUAGE: English

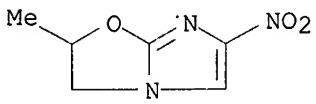
OTHER SOURCE(S): CASREACT 101:211044
IT 73332-75-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 73332-75-9 CAPLUS
CN Imidazo[2,1-b]oxazole, 2,3-dihydro-2-methyl-6-nitro- (9CI) (CA INDEX NAME)



X Same as #12

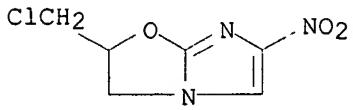
L3 ANSWER 14 OF 15 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1981:174982 CAPLUS <<LOGINID::20061101>>
DOCUMENT NUMBER: 94:174982
TITLE: Potential radiosensitizing agents. 2. Synthesis and biological activity of derivatives of dinitroimidazole with oxiranes
AUTHOR(S): Sehgal, Raj K.; Webb, Matthew W.; Agrawal, Krishna C.
CORPORATE SOURCE: Sch. Med., Tulane Univ., New Orleans, LA, 70112, USA
SOURCE: Journal of Medicinal Chemistry (1981), 24(5), 601-4
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 94:174982
IT 73332-75-9P 73332-76-0P 73332-77-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and radiosensitization activity of)
RN 73332-75-9 CAPLUS
CN Imidazo[2,1-b]oxazole, 2,3-dihydro-2-methyl-6-nitro- (9CI) (CA INDEX NAME)

IDS



X Same as #12

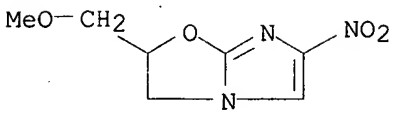
RN 73332-76-0 CAPLUS
CN Imidazo[2,1-b]oxazole, 2-(chloromethyl)-2,3-dihydro-6-nitro- (9CI) (CA INDEX NAME)



X See #12

RN 73332-77-1 CAPLUS
CN Imidazo[2,1-b]oxazole, 2,3-dihydro-2-(methoxymethyl)-6-nitro- (9CI) (CA

INDEX NAME)

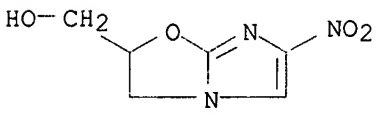


$R^1 = H$ $R^3 = C_1$ Alk

$R^2 = O\text{-}R^3$

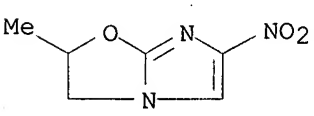
same as 15

IT 73332-78-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation, cyclization, and radiosensitization activity of)
RN 73332-78-2 CAPLUS
CN Imidazo[2,1-b]oxazole-2-methanol, 2,3-dihydro-6-nitro- (9CI) (CA INDEX NAME)



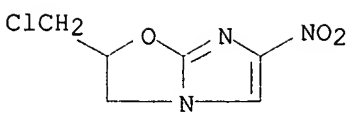
$R^2 = O$
$R^3 = H$

L3 ANSWER 15 OF 15 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1980:163899 CAPLUS <<LOGINID::20061101>>
DOCUMENT NUMBER: 92:163899
TITLE: Novel nitroimidazo[2,1-b]oxazole formation from reaction of 2,4(5)-dinitroimidazole with oxiranes
AUTHOR(S): Sehgal, Raj K.; Agrawal, Krishna C.
CORPORATE SOURCE: Sch. Med., Tulane Univ., New Orleans, LA, 70112, USA
SOURCE: Journal of Heterocyclic Chemistry (1979), 16(7), 1499-500
CODEN: JHTCAD; ISSN: 0022-152X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 92:163899
IT 73332-75-9P 73332-76-0P 73332-77-1P
73332-78-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 73332-75-9 CAPLUS
CN Imidazo[2,1-b]oxazole, 2,3-dihydro-2-methyl-6-nitro- (9CI) (CA INDEX NAME)

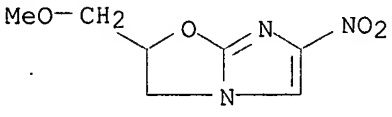


see #12

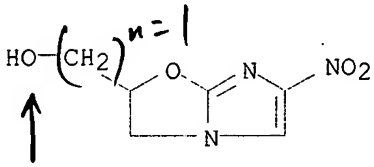
RN 73332-76-0 CAPLUS
CN Imidazo[2,1-b]oxazole, 2-(chloromethyl)-2,3-dihydro-6-nitro- (9CI) (CA INDEX NAME)



RN 73332-77-1 CAPLUS
CN Imidazo[2,1-b]oxazole, 2,3-dihydro-2-(methoxymethyl)-6-nitro- (9CI) (CA INDEX NAME)



RN 73332-78-2 CAPLUS
CN Imidazo[2,1-b]oxazole-2-methanol, 2,3-dihydro-6-nitro- (9CI) (CA INDEX NAME)



$R^2 = OR^3$

$R^3 = H$, Me (C1-6 alkyl)